

Proceedings of the Indian Academy of Sciences (Chemical Sciences)

Volume 99, 1987

CONTENTS

Special issue on Trends in Theoretical Chemistry

Foreword 1

Quantum theory and mathematical methods

Wigner-Weisskopf atom and quantum stochastic dilations
Kalyan B Sinha 3-8

On the use of generalized Euler transformation in handling divergent series
Kamal Bhattacharyya 9-20

Quantum chemistry and quantum biology

Quantum chemistry in phase space: Some current trends
Swapan K Ghosh 21-28

A viable alternative to the unitary group approach in quantum chemistry
A Mukhopadhyay 29-37

Radiative interactions in diatomic molecules
Dilip K Bhattacharyya and Pritha Mitra 39-46

On scattering from fractal lattices
Harjinder Singh and P K Chattaraj 47-51

Trajectory approach to the calculation of sticking probability
K L Sebastian 53-60

On the development of many-body theories for intramolecular dynamics
M Durga Prasad 61-65

How can density functional theory be excited from the ground state?
B M Deb and P K Chattaraj 67-72

The iterative hole-particle method for excited states calculation: Application to tetratomic thiocarbonyls	<i>Manas Banerjee and Asit Kumar Chandra</i>	73–82
On the use of dipole moment as a collective coordinate in constrained variational calculations	<i>P Khan, K K Das and S P Bhattacharyya</i>	83–89
A valency method for the prediction of geometry of molecular excited states	<i>Prabha Siddarth and M S Gopinathan</i>	91–95
Metastable lifetimes and fast chemical reactions	<i>S R Shenoy</i>	97–103
The fragment molecular orbital approach in organometallic reactivity. Reactions of the binuclear complexes	<i>E D Jemmis and B V Prasad</i>	105–111
Molecular electrostatic potential mapping using a dipole	<i>Anil Kumar and P C Mishra</i>	113–118
Nucleoside antibiotics: Conformation and biological activity	<i>Anil Saran</i>	119–128
Statistical mechanics		
Trends in the equilibrium theory of polyatomic fluids	<i>Bhalachandra L Tembe</i>	129–135
<hr/>		
Inorganic and Analytical		
Synthesis and spectroscopic investigations of complexes of lanthanide nitrates with 5-nitroisoquinoline-2-oxide	<i>N Rajasekar</i>	137–141
Inter-ligand stacking interactions in some <i>o</i> -phenanthroline amino acid biligand complexes	<i>Shikha Bajpai and M C Saxena</i>	143–147
Catalytic decomposition of hydrogen peroxide on fine particle ferrites and cobaltites	<i>Tanu Mimani, P Ravindranathan and K C Patil</i>	209–215
Tetrad effects in mixed ligand lanthanide chelates. Part I: Lanthanide, EDTA/NTA, IMDA ternary systems	<i>Sangeeta Verma and M C Saxena</i>	217–222
2-Oximinodimedone monoguanyldiazide as spectrophotometric reagent for determination of iron	<i>J J Berzas Nevado, A Espinosa Mansilla, I M Plata and F Salinas</i>	223–229
Application of galvanic stripping analysis to trace determination of tin	<i>S Jaya, T Prasada Rao and G Prabhakara Rao</i>	231–236

Schiff bases of nickel(II), copper(II) porphyrins and dibenzo-18-crown-6 interspersed <i>bis</i> -metal porphyrins. Protonation studies <i>G Bhaskar Maiya and V Krishnan</i>	283-296
Interaction of rare earth metal ions with nucleosides – a study of binary and ternary systems in solution <i>P Rabindra Reddy, P R Prasad Reddy and M Harilatha Reddy</i>	297-303
Synthesis and spectral characterization of dioxouranium(VI) complexes of salicylhydrazine and acetone salicylhydrazone <i>R A Lal</i>	305-310
X-ray structure of dihydrazinium uranyl dioxalate monohydrate <i>M D Poojary and K C Patil</i>	311-315
Electrochemical study of triphenyltin piperidyl dithiocarbamate <i>Shubhra Chandra, B D James and R J Magee</i>	317-325
Organic	
Some benzimidazole amide complexes of ruthenium(II) <i>T Satyanarayana and K Veera Reddy</i>	237-242
A new synthesis of (\pm) and (+)-2,6,7,7a-tetrahydro-1 β -hydroxy-4-formyl-7a β -methylindenes <i>R Saibaba, D K Banerjee, T R Kasturi and J Mukherjee</i>	327-340
Rapid chemical synthesis of d(CACGTG) in milligram amounts by solution phase phosphotriester chemistry <i>G V Rajendra Kumar, N Sivakamisundari and K N Ganesh</i>	341-350
Physical and Theoretical	
An approximate theory of large molecules and molecular complexes <i>G P Das and K Basu-Ghose</i>	149-157
<i>Ab initio</i> calculations of fundamental frequencies for isomeric difluorobenzenes <i>O P Singh, J S Yadav and R A Yadav</i>	159-166
Resonance Raman studies of tetraphenylporphinato manganese(III) chloride <i>M Sarkar and A L Varma</i>	167-186
Binding of ketoprofen with bovine serum albumin <i>Meenakshi Maruthamuthu and Sankaran Kishore</i>	187-193
A new method of determining solubility of salts and simple salt mixtures at higher temperatures (0 to 200°C) and up to 100 bar pressure <i>V R K S Susarla, A Eber and E U Franck</i>	195-202

Studies on binary and ternary complexes of Co(II) and Ni(II) ions <i>J K Nepal and S N Dubey</i>	203–206
On the behaviour of small clusters near the spinodal decomposition <i>Biman Bagchi</i>	243–252
Studies on interaction of ions with nitromethane and acetonitrile using CNDO/force method <i>R Brakaspathy and Surjit Singh</i>	253–260
One-electron reduction of thionine studied by pulse radiolysis <i>S N Guha, P N Moorthy, K Kishore, D B Naik and K N Rao</i>	261–271
Binding of naproxen to bovine serum albumin and tryptophan-modified bovine serum albumin <i>Meenakshi Maruthamuthu and S Kishore</i>	273–279
Pulse radiolysis study of one electron oxidation of thionine in aqueous solutions <i>S Kishore, S N Guha and P N Moorthy</i>	351–359
Electronic structure of biopolymers – solid state aspects <i>A K Bakhshi</i>	361–392
Binding of 1-anilinonaphthalene-8-sulphonate to poly(N-vinyl-2-pyrrolidone) <i>Meenakshi Maruthamuthu and E Subramanian</i>	393–402
Crystal structure of hirudonine sulphate – a rare polyamine <i>M Nethaji and Vasantha Pattabhi</i>	403–411
Enthalpies of hydrogen-bonded butylamine-chloroform complexes <i>Gopal Pathak and Shirish Pradhan</i>	413–417
Conformations of dibenzylideneacetone: An IR spectroscopic study <i>G Venkateshwarulu and B Subrahmanyam</i>	419–424
Rapid Communication	
On the $\pi^2S + \pi^2S$ pathways toward $[n]$ -prismanes <i>E D Jemmis and G Leela</i>	281–282
Erratum	207
Subject Index	425
Author Index	431